Percentage Yield Calculations

The yield in a chemical reaction is the quantity of product obtained. The actual yield can be compared, as a percentage, with the theoretical.

Worked Example 1

5g of methanol reacts with excess ethanoic acid to produce 9.6g of methyl ethanoate. Calculate the percentage yield.

Step 1: determine the theoretical yield (the quantity expected from the balanced equation)

$$CH_3OH + CH_3COOH \longrightarrow CH_3OOCCH_3$$

1 mol → 1 mol

$32g \longleftrightarrow 74g$

$5g \longrightarrow \frac{74 \times 5}{32} = 11.56g$

Theoretical Yield = **11.56g**

Step 2: The actual yield is always given in the question.

Actual yield = **9.6g**

Step 3: Percentage yield = $\frac{9.6}{11.56} \times 100$

= **83%**

The percentage yield is a very important consideration for industrial chemists. They must take account of cost of raw materials, plant-running costs etc. If the yield of product is not sufficient enough to cover the costs of production then the process would not be considered to be economically viable.

Atom Economy

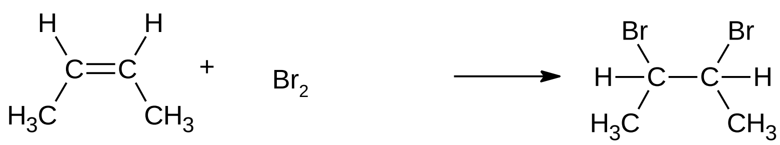
Atom economy is a measure of the proportion of reactant atoms which are incorporated into the desired product of a chemical reaction.

Calculation of atom economy therefore also gives an indication of the proportion of reactant atoms forming waste products.

$$\% \text{ atom economy} = \frac{\text{Mass of desired product(s)}}{\text{Total mass of reactants}} \times 100$$

In developing an atom economical reaction pathway the industrial chemist may well prefer rearrangement and addition reactions over less environmental friendly substitution and elimination reactions.

Example 1: Addition reaction – halogenation of an alkene



(Z)-but-2-ene	Bromine	2,3-dibromobutane
C_4H_8	Br_2	$C_4H_8Br_2$
1mol	1mol	1mol
(12 x 4) + (8 x 1)	2 x 79.9	(12 x 4) + (8 x 1) + (79.9 x 2)
= 56g	= 159.8g	= 215.8g

Total mass of reactants = 56 g + 159.8 g = 215.8 g
(Note: Product mass is also 215.8 g)

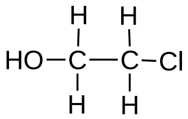
Mass of desired product (2,3-dibromobutane) = 215.8 g

$$\% \text{ atom economy} = \frac{\text{Mass of desired product(s)}}{\text{Total mass of reactants}} \times 100$$

$$\% \text{ atom economy} = \frac{215.8}{215.8} \times 100 = \mathbf{100\%}$$

This process is 100% atom efficient, with all the reactant atoms included within the desired product.

Example 2: Elimination reaction

2  + $Ca(OH)_2$ ⟶

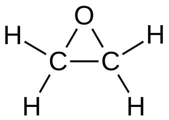
2-chloroethanol
C_2H_5OCl
2mol
2[(12 x 2) + (5 x 1) + 16 + 35.5]

= 161g

Calcium hydroxide
$Ca(OH)_2$
1mol
40 + 2(16 +1)

= 74g

Desired Product

2  +

ethylene oxide
C_2H_4O
2mol
2[(12 x 2) + (4 x 1) + 16]

= 88g

Waste Products

$CaCl_2$ + $2H_2O$

Calcium chloride
$CaCl_2$
1mol
40 + (2 x 35.5)

= 111g

Water
H_2O
2mol
2 [(2 x 1) + 16]

= 36g

Total mass of reactants = 161 g + 74 g = 235 g
(Note: Total product mass = 235 g)

Mass of desired product ethylene oxide = 88 g

$$\% \text{ atom economy} = \frac{\text{Mass of desired product(s)}}{\text{Total mass of reactants}} \times 100$$

$$\% \text{ atom economy} = \frac{88}{235} \times 100 = \mathbf{37.4\%}$$

This elimination reaction is therefore only 37.4% atom efficient, with the remaining 62.6% in the form of unwanted waste products (calcium chloride and water).